

CLAIMS

1. In a method of identifying an analysis-objective sugar chain structure using a mass spectrometer by comparing a measured MS3 fragment pattern with a reference MS3 fragment pattern stored in a database, where the measured MS3 fragment pattern is a fragmentation pattern of each MS2 fragment ion included in a measured MS2 fragment pattern obtained by subjecting the analysis-objective sugar chain to a fragmentation mass spectroscopy,

the method of identifying a sugar structure characterized in that, among a plurality of MS2 fragment ions included in a measured MS2 fragment pattern, a fragmentation mass spectroscopy is performed on only selected MS2 fragment ions, where each of the selected MS2 fragment ions has a plurality of reference MS3 fragment patterns stored in a database whose mutual similarity index is the same as or smaller than a predetermined value, wherein the plurality of reference MS3 fragment patterns have the same precursor ion mass to charge ratio as that of the selected MS2 fragment ion.

2. The method of identifying a sugar chain structure according to claim 1, wherein reference MS4 fragment patterns or MS_n reference fragment patterns from further fragmentation are further stored in the database, identification of a sugar chain structure is performed by comparing them with a measured MS4 fragment pattern or an MS_n measured fragment pattern from further fragmentation, and, in the same manner as described above, only measured MS_n fragment ions having mutual similarity index between a plurality of reference MS_n+1 fragment patterns of not higher than a predetermined value are subjected to a further fragmentation mass spectroscopy.

3. In a method of identifying an analysis-objective sugar chain structure using a mass spectrometer by comparing a measured MS3 fragment pattern with a reference MS3 fragment pattern stored in a database, where the measured MS3 fragment pattern is a fragmentation pattern of each MS2 fragment ion included in a measured MS2 fragment pattern obtained by subjecting the analysis-objective sugar chain to a fragmentation mass spectroscopy,

the method of identifying a sugar structure characterized in that, among a plurality of MS2 fragment ions included in a measured MS2 fragment pattern, fragmentation mass spectroscopies are performed in the order of smaller to larger mutual similarity index of the a plurality of MS3 fragment patterns stored in a database, wherein the plurality of reference MS3 fragment patterns have the same precursor ion mass to charge ratio as that of the selected MS2 fragment ion.

4. The method of identifying a sugar chain structure according to claim 3, wherein reference MS4 fragment patterns or MS_n reference fragment patterns from further fragmentation are further stored in the database, identification of a sugar chain structure is performed by comparing with a measured MS4 fragment pattern or an MS_n measured fragment pattern from further fragmentation, and, in the same manner as described above, only measured MS4 fragment ions having mutual similarity index between a plurality of reference MS_n+1 fragment patterns of not higher than a predetermined value are subjected to a further fragmentation mass spectroscopy.

5. The method of identifying a sugar chain structure according to any one of claims 1 to 4, wherein the mutual similarity index between the aforementioned reference MS_n+1 fragment patterns is stored in the database by associating with a mass to charge

ratio of the precursor ion.

6. The method of identifying a sugar chain structure according to any one of claims 1 to 5, wherein only MS_n fragment ions having a peak intensity in a measured
5 MS_n fragment pattern of not lower than a predetermined value are subjected to the identification method.

7. The method of identifying a sugar chain structure according to any one of claims 1 to 6, wherein a theoretical composition of a sugar chain is calculated from a
10 measured MS_n fragment pattern and, based on this, among reference MS_{n+1} fragment patterns stored in the database, patterns to be compared are restricted in advance.

8. The method of identifying a sugar chain structure according to any one of claims 1 to 7, wherein the fragmentation energy of the fragmentation mass spectroscopy
15 is set to be not smaller than a predetermined value depending on the precursor ion.

9. The method of identifying a sugar chain structure according to claim 8, wherein the predetermined value of fragmentation energy is stored in the database.

20 10. The method of identifying a sugar chain structure according to any one of claims 1 to 9, wherein the similarity index between two fragment patterns is determined by the following method:

a) in a first fragment pattern, peaks having a mass to charge ratio in a predetermined range are grouped together and, among those peaks, the peak having the
25 highest intensity is adopted as the peak representing the range.

b) in a second fragment pattern, a representative peak is selected by the same ranging as that described above.

c) letting the Euclidean distance between two vectors composed of the elements of intensities of the representative peaks in respective ranges of both fragment patterns as a
5 dissimilarity index, and similarity index is determined based on the dissimilarity index.

11. The method of identifying a sugar chain structure according to claim 10, wherein regarding a second fragment pattern having the dissimilarity index of not higher than a predetermined value relative to a first fragment pattern, the aforementioned
10 procedure is repeated by exchanging first and second patterns to calculate a second dissimilarity index, and the similarity index is determined based on the second dissimilarity index.

12. A mass spectrometer for analyzing a sugar chain, which comprises:
15 a mass spectroscopy part equipped with a means for holding and fragmenting an ion,
a database part in which MS_n fragment patterns of known sugar chains are stored,
and
a data processing part for controlling the mass spectrometer based on the method
20 as defined in any one of claims 1 to 11 and identifying the analysis-objective sugar chain.

13. A program for carrying out the method as defined in any one of claims 1 to 11.